4.2 Semiconductor-Semiconductor heterojunctions

4.2.1 Band offset models

In section 2.1.3, we have introduced the concept of heterojunction band offsets. Three types of the band offset exist, which are straddling (type I), staggered (type II) or broken-gap (type III) in character. In this section, we will discuss some models in order to provide some useful insight how the band offsets are formed at the heterojunction interface.

1. Andeson's model

For an ideal abrupt heterojunction without interface traps, Aderson (1962) proposed an energy band model, which is very similar to the Schottky-Mott model for metal-semiconductor junction. According to his model the energy bands in both semiconductor materials constituting a heterostructure are not affected each other. He then assumed that the vacuum energy level is continuous and, hence, the conduction band offset is determined by the difference of electron affinities, i.e.,

$$\Delta E_c = \chi_1 - \chi_2 \tag{4.2.1}$$

The valence band offset is then given by

$$\Delta E_v = \Delta E_g - \Delta E_c \tag{4.2.2}$$

or

$$\Delta E_v = \Delta E_g - \chi_1 + \chi_2, \tag{4.2.3}$$

where, ΔE_g is the energy gap discontinuity. However, this model is in disagreement with the experimental data.

2. Tersoff's model

Tersoff postulated in 1984 that the band offset in the heterojunctions are controlled by the same mechanism as the barrier height in the Schottky barrier diodes. This mechanism is the electron tunneling from one material into the energy gap of the other semiconductor at the heterointerface, leading to the formation of the interfacial dipole layer. The conduction band offset can then be related to the difference in the Schottky barrier heights for the two semiconductor materials forming the heterojunction

$$\Delta E_c = q(\Phi_{b1} - \Phi_{b2}). \tag{4.2.4}$$

Generally, a good correlation has been found when comparing the theoretically predicted band offset values using this model with experimental results for lattice matched heterojunctions, e.g., GaAs/$Al_xGa_{1-x}As$ (x=0 - 1).

3. Role of the lattice strain

No mater how accurate they are, the above two models can only be used to describe the lattice matched (i.e., two semiconductors forming a heterojunction have the nearly same lattice constant in plane, e.g, GaAs/Ge and GaAs/AlGaAs) heterostructures.

If the difference of the lattice constants in plane for two semiconductors is small (e.g., $\lesssim 5\%$), using modern epitaxial growth techniques materials (MBE or LTCVD) a thin layer of one material can be grown on the substrate of another material without generation of misfit dislocations. The in plane lattice constant $a_{//}$ of the thin layer will be constrained to match with that of the substrate (*biaxial strain*) while the perpendicular lattice constant $a_{\perp}$ will be either extended or contracted (*uniaxial strain*). At the same time, the fractional volume change also leads to the *hydrostatic strain.* Such a growth mode is call pseudomorphic or commensurate growth. The critical thickness to keep pseudomorphic growth is limited by the lattice mismatch (in term of the lattice strain) between two semiconductors, and is also dependent on the growth temperature. Above this critical thickness limit, the lattice

stain in the heterojunction structures will be released, instead a large density of misfit dislocations will be formed at the heterojunction interface.

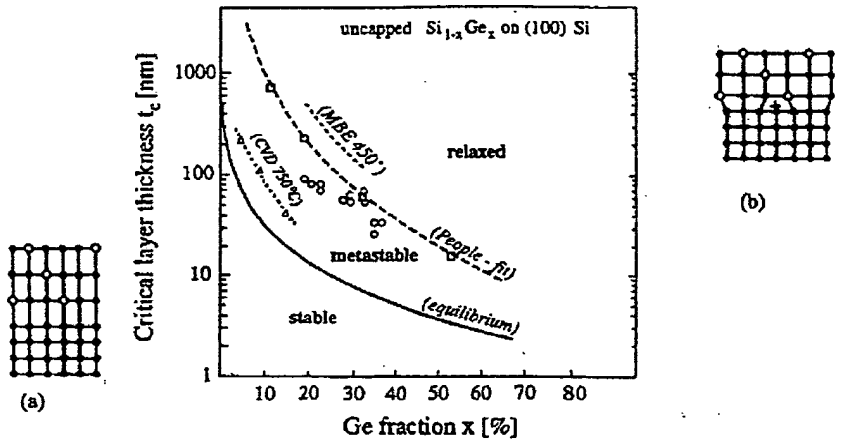

Fig. 4.2.1 The critical thickness of SiGe pseudomorphic growth vs. Growth temperature and Ge fraction. Insert figures show schematically (a) a strained, and (b) a relaxed heterostructure

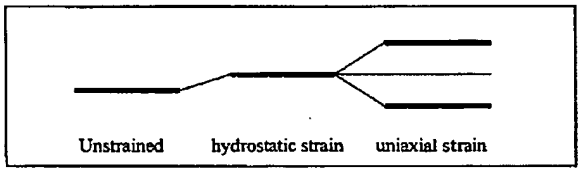

Fig. 4.2.2 Schematic representation of the effect of strain on a triply degenerate band

The strain in the heterostructure has tow main effects on the band structure of a semiconductor: hydrostatic strain due to the volume change of the strained layer shifts the energetic position of a band, and uniaxial strain splits degenerate bands. The band offsets of a strained heterojunction do not follow the bulk band properties of the respective semiconductor. In particular, different configurations of strain (compressive or tensile) will result in different spilt shifts, eventually different band offset values. An example of strained Si/SiGe heterostructures is shown in Fig. 4.2.2

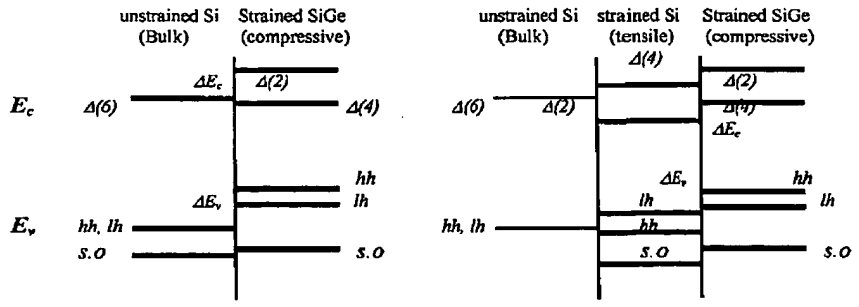

Fig. 4.2.3 Strain dependence of the band offsets for various Si/SiGe heterojunctions

4.2.2 Built-in voltage and space charge region across a heterojunction interface